Novel, Light-Element Nanostructured Materials for Hydrogen Storage (New FY 2004 Project)

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Objectives

To demonstrate the operation of a nanostructure-based hydrogen storage tank which meets the DOE cost goals of $5/kW-hr

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year R,D&D Plan:

- A. Cost
- B. Weight and Volume
- M. Hydrogen Capacity and Reversibility

Approach

This project will develop and prototype a new hydrogen storage technology based on low-temperature physisorption of hydrogen on nanostructured materials based on light elements. The Nanomix team will develop and test new materials and scale them up to prototype testing. The materials will be the heart of a simple storage system that takes advantage of the inherent thermodynamic properties of hydrogen and promises to surpass competing technologies in overall system performance. Starting with activated carbon, Nanomix will design and construct a pilot-scale prototype to define and study critical operating parameters such as temperature, pressure, refueling time, and dormancy. The research and development effort will identify new materials with appropriate heats of adsorption using computational tools, synthesize and test both known and new candidate materials, develop high surface area forms, construct a storage tank prototype, and test the tank with quantities of candidate materials that emerge successfully from the preceding materials development project.

This three-year project includes seven separate tasks:

Task 1. Planning and Management: Prepare a project management plan that addresses organization, schedule budget, procurement, health & safety, data quality and reporting. Participate in DOE Hydrogen, Fuel Cells and Infrastructure Technologies Program meetings, etc.

Task 2. Computational Design and Screening: Identify new candidate materials for hydrogen adsorption; conduct screening level ab initio calculations of the binding energy of hydrogen; perform density functional calculations on promising candidates; and predict composition, structure and

stability and project cost of production and toxicity. Complete analysis of two groups in the first year and identify at least 2 new materials.

Task 3. Experimental Verification: Procure or synthesize small quantities of nanostructured materials for screening; characterize hydrogen storage properties - binding energy and coverage over a range of temperatures; and select high potential materials. Complete verification of at least two new materials in the first year.

Task 4. Optimize Material for Hydrogen Storage: Synthesize very high surface area samples and conduct engineering measurements of hydrogen storage properties. Complete synthesis of B_2O_3 and at least one new material in the first year.

Task 5. Pilot Material Synthesis / Production: Evaluate pilot-scale and larger process feasibility and production costs; synthesize B_2O_3 or another material for testing in the first year.

Task 6. Prototype Testing: Design and construct a prototype H_2 storage tank to test material and operating parameters; test high surface area carbon structures in the first year.

Task 7. Reporting and Deliverables: Submit quarterly and annual project reports.